cis-Cyclohex-4-en-1,2-dicarboxylic acid, dodecyl 2-ethylhexyl ester

Inchi: InChI=1S/C28H50O4/c1-4-7-9-10-11-12-13-14-15-18-22-31-27(29)25-20-16-17-21-26(25

InchiKey: KUWQZPAVOPISBB-UHFFFAOYSA-N

Formula: C28H50O4

SMILES: CCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCC(CC)CCCC

Mol. weight [g/mol]: 450.69

Physical Properties

Property code	Value	Unit	Source
gf	-238.70	kJ/mol	Joback Method
hf	-1024.37	kJ/mol	Joback Method
hfus	64.45	kJ/mol	Joback Method
hvap	96.26	kJ/mol	Joback Method
log10ws	-8.29		Crippen Method
logp	7.792		Crippen Method
mcvol	405.100	ml/mol	McGowan Method
pc	772.46	kPa	Joback Method
rinpol	2990.00		NIST Webbook
rinpol	2990.00		NIST Webbook
tb	1006.22	K	Joback Method
tc	1235.53	K	Joback Method
tf	538.54	K	Joback Method
vc	1.563	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1443.30	J/mol×K	1006.22	Joback Method
cpg	1463.06	J/mol×K	1044.44	Joback Method
cpg	1480.80	J/mol×K	1082.66	Joback Method
cpg	1496.57	J/mol×K	1120.87	Joback Method
cpg	1510.43	J/mol×K	1159.09	Joback Method
cpg	1522.44	J/mol×K	1197.31	Joback Method
cpg	1532.67	J/mol×K	1235.53	Joback Method
dvisc	0.0004473	Pa×s	538.54	Joback Method

dvisc	0.0001966	Pa×s	616.49	Joback Method
dvisc	0.0001039	Pa×s	694.43	Joback Method
dvisc	0.0000625	Pa×s	772.38	Joback Method
dvisc	0.0000412	Pa×s	850.33	Joback Method
dvisc	0.0000292	Pa×s	928.27	Joback Method
dvisc	0.0000218	Pa×s	1006.22	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382639&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume